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PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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                     Welcome to STN International
                 Web Page for STN Seminar Schedule - N. America
NEWS
NEWS
         JAN 02
                 STN pricing information for 2008 now available
NEWS
         JAN 16
                 CAS patent coverage enhanced to include exemplified
                 prophetic substances
NEWS
         JAN 28
                 USPATFULL, USPAT2, and USPATOLD enhanced with new
                 custom IPC display formats
NEWS
         JAN 28
                 MARPAT searching enhanced
NEWS 6
         JAN 28
                 USGENE now provides USPTO sequence data within 3 days
                 of publication
         JAN 28
NEWS
                 TOXCENTER enhanced with reloaded MEDLINE segment
                 MEDLINE and LMEDLINE reloaded with enhancements
NEWS 8
         JAN 28
NEWS 9 FEB 08
                 STN Express, Version 8.3, now available
NEWS 10 FEB 20 PCI now available as a replacement to DPCI
NEWS 11 FEB 25
                 IFIREF reloaded with enhancements
NEWS 12 FEB 25
                 IMSPRODUCT reloaded with enhancements
NEWS 13 FEB 29
                 WPINDEX/WPIDS/WPIX enhanced with ECLA and current
                 U.S. National Patent Classification
                 IFICDB, IFIPAT, and IFIUDB enhanced with new custom
NEWS 14
         MAR 31
                 IPC display formats
NEWS 15
         MAR 31
                 CAS REGISTRY enhanced with additional experimental
NEWS 16
                 CA/CAplus and CASREACT patent number format for U.S.
         MAR 31
                 applications updated
NEWS 17
         MAR 31
                 LPCI now available as a replacement to LDPCI
NEWS 18 MAR 31
                 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 19 APR 04
                 STN AnaVist, Version 1, to be discontinued
NEWS 20 APR 15
                 WPIDS, WPINDEX, and WPIX enhanced with new
                 predefined hit display formats
NEWS 21 APR 28
                 EMBASE Controlled Term thesaurus enhanced
NEWS 22 APR 28
                 IMSRESEARCH reloaded with enhancements
NEWS 23 MAY 30
                 INPAFAMDB now available on STN for patent family
                 searching
         MAY 30
NEWS 24
                 DGENE, PCTGEN, and USGENE enhanced with new homology
                 sequence search option
NEWS 25
         JUN 06
                 EPFULL enhanced with 260,000 English abstracts
NEWS 26
         JUN 06
                 KOREAPAT updated with 41,000 documents
NEWS 27
         JUN 13
                 USPATFULL and USPAT2 updated with 11-character
                 patent numbers for U.S. applications
NEWS 28
         JUN 19
                 CAS REGISTRY includes selected substances from
                 web-based collections
NEWS 29
         JUN 25
                 CA/CAplus and USPAT databases updated with IPC
                 reclassification data
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NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3, AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

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=> fil reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 18:44:44 ON 26 JUN 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 25 JUN 2008 HIGHEST RN 1030702-50-1 DICTIONARY FILE UPDATES: 25 JUN 2008 HIGHEST RN 1030702-50-1

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

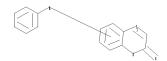
Please note that search-term pricing does apply when conducting SmartSELECT searches.

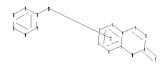
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

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chain nodes :
11 20
ring nodes :
1 2 3 4 5 6 7 8 9 10 14 15 16 17 18 19
chain bonds :
9-11 18-20
ring bonds :
1-6 1-2 2-3 3-4 4-5 4-7 5-6 5-10 7-8 8-9 9-10 14-15 14-19 15-16 16-17
17-18 18-19
exact/norm bonds :
4-7 5-10 7-8 8-9 9-10 9-11 18-20
normalized bonds :
1-6 1-2 2-3 3-4 4-5 5-6 14-15 14-19 15-16 16-17 17-18 18-19
isolated ring systems :
containing 1 :

G1:N,CH

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:CLASS 21:Atom

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

G1 N, CH

Structure attributes must be viewed using STN Express query preparation.

2 ANSWERS

=> s 11 sss sam SAMPLE SEARCH INITIATED 18:45:20 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -33549 TO ITERATE

6.0% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** **COMPLETE** BATCH

PROJECTED ITERATIONS: 660029 TO 681931 PROJECTED ANSWERS: 323 TO 1017

L2 2 SEA SSS SAM L1

=> d scan

REGISTRY COPYRIGHT 2008 ACS on STN L2 2 ANSWERS

ΙN 2,3-Quinoxalinedione, 6-[amino(2-iodophenyl)methyl]-1,4-dihydro-

MFC15 H12 I N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

REGISTRY COPYRIGHT 2008 ACS on STN L2 2 ANSWERS

ΙN 2(1H)-Quinolinone, 6-[(3,4-dichlorophenyl)[4-[(2-methoxyethyl)amino]-1piperidinyl]methyl]-3-ethyl-

MF C26 H31 C12 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s 11 sss full FULL SEARCH INITIATED 18:45:50 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 678156 TO ITERATE

100.0% PROCESSED 678156 ITERATIONS SEARCH TIME: 00.00.06

390 ANSWERS

L3 390 SEA SSS FUL L1

=> d scan

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2-Quinoxaline carboxylic acid, 7-benzoyl-3,4-dihydro-3-oxo-, ethyl ester MF C18 H14 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-(isocyanatophenylmethyl)-3-methyl-

MF C18 H14 N2 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN Benzoic acid, 4-[(1,2-dihydro-3-methyl-2-oxo-6-quinolinyl)hydroxymethyl]-, ethyl ester

MF C20 H19 N O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[(2,4-difluorophenyl)[4-[(2-methoxyethyl)amino]-1-piperidinyl]methyl]-3-ethyl-

MF C26 H31 F2 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

MF C27 H32 F3 N3 O3

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H) -Quinoxalinone, 7-[2-(4-chlorophenyl)-2-(1H-imidazol-1-yl)ethyl]-3-ethyl-

MF C21 H19 C1 N4 O

$$\begin{array}{c|c} & C1 \\ \hline \\ N & CH-CH_2 \\ \hline \\ N & Et. \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[(R)-1H-1,2,4-triazol-1-yl[4-(trifluoromethyl)phenyl]methyl]-, hydrobromide (1:1)

MF C19 H13 F3 N4 O . Br H

Absolute stereochemistry.

• HBr

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]-, (S)- (9CI)

MF C19 H13 F3 N4 O

Absolute stereochemistry. Rotation (+).

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinoxalinone, 1-amino-6-(1H-imidazol-1-ylphenylmethyl)-3-methyl-

MF C19 H17 N5 O

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2,3-Quinoxalinedione, 6-[amino(4-methylphenyl)methyl]-1,4-dihydro-

MF C16 H15 N3 O2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN INDEX NAME NOT YET ASSIGNED

MF C21 H15 N3 O7

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[(2,3-dihydro-1,4-benzodioxin-6-yl)[1-[2-(4-methoxyphenyl)ethyl]-4-piperidinylidene]methyl]-3-ethyl-

MF C34 H36 N2 O4

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H) -Quinolinone, 3-methyl-6-[1-phenyl-3-(1-piperidinyl)propyl]-

MF C24 H28 N2 O

$$\begin{array}{c|c} & & & \text{Ph} & & \text{H} & \text{N} \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[(2,3-dihydro-1,4-benzodioxin-6-yl)][[1-(phenylmethyl)-3-piperidinyl]amino]methyl]-3-ethyl-

MF C32 H35 N3 O3

CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 390 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN

IN 2(1H)-Quinolinone, 6-[(2,3-dihydro-1,4-benzodioxin-6-yl)[1-[(2E)-3-phenyl-2-propen-1-yl]-4-piperidinyl]methyl]-3-ethyl-

MF C34 H36 N2 O3

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):fil cap 'FIL CAP' IS NOT VALID HERE

To display more answers, enter the number of answers you would like to see. To end the display, enter "NONE", "N", "0", or "END". HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> fil cap

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 179.74 179.95

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FILE COVERS 1907 - 26 Jun 2008 VOL 148 ISS 26 FILE LAST UPDATED: 25 Jun 2008 (20080625/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

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(FILE 'HOME' ENTERED AT 18:44:37 ON 26 JUN 2008)

FILE 'REGISTRY' ENTERED AT 18:44:44 ON 26 JUN 2008

L1 STRUCTURE UPLOADED

L2 2 S L1 SSS SAM L3 390 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 18:47:06 ON 26 JUN 2008

=> s 13 and (py<2005)

37 L3

25085366 PY<2005

L4 28 L3 AND (PY<2005)

=> d 1-28 ibib abs hitstr

L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:430796 CAPLUS

DOCUMENT NUMBER: 141:7139

TITLE: Preparation of indolylquinoxalinones for treating

hyperproliferative disorders and diseases associated

with angiogenesis

INVENTOR(S): Ladouceur, Gaetan H.; Bear, Brian; Bi, Cheng;

Brittelli, David R.; Burke, Michael J.; Chen, Gang; Cook, James; Dumas, Jacques; Sibley, Robert; Turner,

Michael R.

PATENT ASSIGNEE(S): Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 217 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2004043950 A1 20040527 WO 2003-US36003 20031110 <-W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,

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             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
             OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
             TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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PRIORITY APPLN. INFO.:
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                                                                     20030630
                                             WO 2003-US36003
                                                                  W
                                                                     20031110
                         MARPAT 141:7139
OTHER SOURCE(S):
```

GΙ

AB The invention relates to title compds. I [wherein Ar = 6-membered aromatic ring containing 0-2 N atoms; R1 and R2 = independently H, halo, CF3, acyl, piperidinyl, piperazinyl, morpholinyl, or (un)substituted alkyl, alkoxy, amino, pyrrolidinyl, Ph, etc.; R3 = H, alkyl, OH, NO2, NH2, alkylamino, alkoxyamino, or (un) substituted benzoylamino; R4 = H, OH, halo, CN, acyl, sulfamoyl, trialkylsiloxy, tetrazolyl, thienyl, pyrrolyl, pyrimidinyl, oxazolyl, furanyl, or (un)substituted alkyl, alkenyl, alkynyl, alkoxy, amino, oxadiazolyl, Ph, pyridyl(oxy), carbamoyl; R11 and R12 = independently H, F, or Cl with the proviso that when one of R11 and R12 = $\frac{1}{2}$ F or Cl, the other must be H; and pharmaceutically acceptable salts and esters thereof]. The invention also relates to the use of I and their pharmaceutical compns. for treating hyperproliferative disorders and diseases associated with angiogenesis (no data). Examples include representative syntheses for compds. of the invention, pharmaceutical compns. comprising them, and tumor model assays (no specific data given). For instance, N-Boc-indole was coupled with di-Me oxalate using t-BuLi to give tert-Bu 2-[methoxy(oxo)acetyl]-1H-indole-1-carboxylate (72%). Cyclization of the dione with 1,2-phenylenediamine in AcOH afforded the quinoxalinone II (77%). ΙT

694531-84-5P 694531-85-6P 694531-86-7P

694531-90-3P 694531-93-6P 694531-94-7P

694532-04-2P 694532-29-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(antiproliferative and angiogenesis inhibitor; preparation of indolylquinoxalinones for treating hyperproliferative disorders and diseases associated with angiogenesis)

RN 694531-84-5 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-[[(3S)-3-(dimethylamino)-1-pyrrolidinyl]carbonyl]-1H-indol-2-yl]-6-benzoyl- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 694531-85-6 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-[[4-(2-methoxyethyl)-1-piperazinyl]carbonyl]-1H-indol-2-yl]-6-benzoyl- (CA INDEX NAME)

RN 694531-86-7 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(1-piperidinylcarbonyl)-1H-indol-2-yl]-6-benzoyl- (CA INDEX NAME)

RN 694531-90-3 CAPLUS

CN 1H-Indole-5-carboxamide, 3-amino-2-(6-benzoyl-3,4-dihydro-3-oxo-2-quinoxalinyl)-N-(2-methoxyethyl)-N-methyl- (CA INDEX NAME)

RN 694531-93-6 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(1-pyrrolidinylcarbonyl)-1H-indol-2-yl]-6-benzoyl- (CA INDEX NAME)

$$\begin{array}{c|c} O & H_2N & O \\ \hline Ph-C & N & H \\ \hline N & O & H \\ \end{array}$$

RN 694531-94-7 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-(1-pyrrolidinylcarbonyl)-1H-indol-2-yl]-7-benzoyl- (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\$$

RN 694532-04-2 CAPLUS

CN 1H-Indole-5-carboxylic acid, 3-amino-2-(7-benzoyl-3,4-dihydro-3-oxo-2-quinoxalinyl)- (CA INDEX NAME)

RN 694532-29-1 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[3-amino-5-[[(3S)-3-(dimethylamino)-1-pyrrolidinyl]carbonyl]-1H-indol-2-yl]-7-benzoyl- (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:796538 CAPLUS

DOCUMENT NUMBER: 139:323440

TITLE: Preparation of radiolabeled quinolines and

quinolinones as metabotropic glutamate receptor mGluR1 antagonists for use in positron emission tomography.

INVENTOR(S): Lesage, Anne Simone Josephine; Bischoff, Francois

Paul; Janssen, Cornelus Gerardus Maria; Lavreysen,

Hilde

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 148 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	TENT	NO.			KIND DATE					APPLICATION NO.						DATE				
WO WO			A2 200 A3 200					WO 2	003-	EP32	40		2	326	<					
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		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM_{\bullet}	ZW								
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	R:				•		ES,	•	•		•				•	•	PT,			
							RO,													
	1642				А		2005						-							
	2005		79				2005			JP 2						0030.				
	5354				A		2006			NZ 2					_	0030.				
ΙN	2004						2005			IN 2			_							
	2006				A1		2006			US 2										
	2004						2005			MX 2004-PA9435						20040928				
ZA	A 2004007820						2005	1011		ZA 2	004-	7820			20040928					

NO 2004004635 PRIORITY APPLN. INFO.:

A 20041027

NO 2004-4635 EP 2002-76254

WO 2003-EP3240

20041027 <--A 20020329

W 20030326

OTHER SOURCE(S):

MARPAT 139:323440

GΙ

Radiolabeled title compds. [I, II; X = O, S, C(R6)2, NR7; Y = O, S; R1 = AB (substituted) alkyl, cycloalkyl, cycloalkylalkyl, thienyl, quinolinyl, etc.; R2 = H, halo, cyano, alkyl, amino, heterocyclyl, etc.; R3, R4 = H, halo, OH, cyano, alkyl, alkoxy, etc.; R2R3 = (CH2)3-6, Z4CH2CH2CH2, Z4CH2CH2, etc.; Z4 = O, S, SO2, NR11; R11 = H, alkyl, PhCH2, alkoxycarbonyl; R3R4 = (CH2)4, CH:CHCH:CH; R5 = H, cycloalkyl, piperidinyl, oxothienyl, tetrahydrothienyl, aralkyl, alkoxyalkyl, etc.; R6 = H, aryl, alkyl, aminoalkyl; R7 = amino, OH], were prepared Most preferred are radiolabeled compds. in which the radioactive isotope is selected from 3H, 11C and 18F. The invention also relates to their use in a diagnostic method, in particular for marking and identifying a mGluR1 receptor in biol. material, as well as to their use for imaging an organ, in particular using positron emission tomog. (PET). Thus, title compound (III) was prepared by tritiation of the corresponding bromide in THF using tritium gas and Pd/C catalyst. The purified product showed specific activity of 25 Ci/mmol.

IT 409344-47-4P 409344-48-5P 409344-56-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of radiolabeled quinolines and quinolines as metabotropic glutamate receptor mGluR1 antagonists for use in positron emission tomog.)

RN 409344-47-4 CAPLUS

CN 2(1H)-Quinolinone, 3-ethyl-6-(2-phenylacetyl)- (CA INDEX NAME)

$$Ph-CH_2-C$$

$$O$$

$$Et$$

$$\begin{array}{c|c} \text{OMe} & \text{O} & \text{H} & \text{O} \\ \text{CH}_2 - \text{C} & \text{E} \end{array}$$

RN 409344-56-5 CAPLUS

CN 2(1H)-Quinolinone, 3-ethyl-6-(1-oxo-3-phenylpropyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-C} & & & \\ & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & \\ & &$$

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:235032 CAPLUS

DOCUMENT NUMBER: 139:143344

TITLE: Synthesis and SAR of novel di- and trisubstituted

1,4-dihydroquinoxaline-2,3-diones related to licostinel (Acea 1021) as NMDA/glycine site

antagonists

AUTHOR(S): Zhou, Zhang-Lin; Kher, Sunil M.; Cai, Sui Xiong;

Whittemore, Edward R.; Espitia, Stephen A.; Hawkinson, Jon E.; Tran, Minhtam; Woodward, Richard M.; Weber,

Eckard; Keana, John F. W.

CORPORATE SOURCE: Department of Chemistry, University of Oregon, Eugene,

OR, 97403, USA

SOURCE: Bioorganic & Medicinal Chemistry (2003),

11(8), 1769-1780

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:143344

AB A series of novel di- and trisubstituted 1,4-dihydroquinoxaline-2,3-diones (QXs) related to licostinel (Acea 1021) was synthesized and evaluated as antagonists for the glycine site of the N-methyl-d-aspartate (NMDA) receptor. The in vitro potency of these antagonists was determined by displacement of the glycine site radioligand [3H]-5,7-dichlorokynurenic acid ([3H]DCKA) in rat brain cortical membranes. Structure-activity relationship studies indicate that a cyano group is a good replacement for the nitro group in the 5-position of licostinel while 5-carboxy, 5-ester, 5-ketone and 5-amide derivs. showed reduced potency. 5,6-Cyclized analogs of licostinel also showed significantly reduced potency. Among the trisubstituted QXs investigated, 5-cyano-6,7-dichloro QX and 5-cyano-7-chloro-6-Me QX are the most potent with IC50 values of 32 nM and 26 nM, resp.

IT 573692-50-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and structure-activity relationship of novel di- and trisubstituted 1,4-dihydroquinoxaline-2,3-diones related to licostinel

(Acea 1021) as NMDA/glycine site antagonists)

RN 573692-50-9 CAPLUS

2,3-Quinoxalinedione, 5-benzoyl-7-chloro-1,4-dihydro- (CA INDEX NAME)

C1 N O

CN

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:574925 CAPLUS

DOCUMENT NUMBER: 137:140442

TITLE: Preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-

quinolinones as p38 protein kinase inhibitors

INVENTOR(S): Doherty, James B.; Stelmach, John E.; Chen, Meng-Hsin;

Liu, Luping; Hunt, Julianne A.; Ruzek, Rowena D.; Goulet, Joung L.; Wisnoski, David D.; Natarajan, Swaminathan Ravi; Rupprecht, Kathleen M.; Bao,

Jianming; Miao, Shouwu; Hong, Xingfang

PATENT ASSIGNEE(S): Merck & Co., Inc., USA SOURCE: PCT Int. Appl., 440 pp.

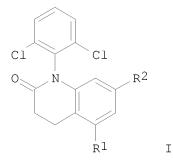
CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	TENT	NO.			KIND DATE						ICAT							
	2002058695 2002058695																	
	W:	GM, LT, PT,	CR, HR, LU, RO,	CU, HU, LV, RU,	CZ, ID, MA, SD,	DE, IL, MD, SE,	AU, DK, IN, MG, SG, ZA,	DM, IS, MK, SI,	DZ, JP, MN, SK,	EC, KE, MW,	EE, KG, MX,	ES, KR, MZ,	FI, KZ, NO,	GB, LC, NZ,	GD, LK, OM,	GE, LR, PH,	GH, LS, PL,	
	RW:	GR,	ΚΖ, ΙΕ,	MD, IT,	RU, LU,	TJ, MC,	MZ, TM, NL,	AT, PT,	BE, SE,	CH, TR,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	
CA	2431	,	~ ,	,	,	,	,	,	,		001-	2431	904		2	0011	214	<
AU	2002	2466	77		A1		2002	0806		AU 2	002-	2466	20011214 <					
AU	2002	2466	77		В2		2006	1116										
EP	1345	603			A1		2003	0924		EP 2	001-	9942	60		2	0011	214	<
	R:	AT, IE,	•	•			ES, RO,	•		•		LI,	LU,	NL,	SE,	MC,	PT,	
JP	2004	5218	92		Τ		2004	0722		JP 2	002-	5590:	29		2	0011	214	<
	2003 6809									US 2	001-	2323	1		2	0011:	217	<
PRIORIT										US 2 WO 2								



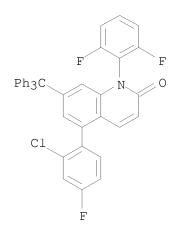
AΒ Title compds. were prepared Thus, 2,6-dibromo-4-methoxytoluene was converted in 5 steps to arylquinolinone I (R1 = Br, R2 = OMe) which was condensed with 2,4-F2C6H3B(OH)2 and the O-demethylated product converted in 4 steps to I (R1 = C6H3F2-2,4, R2 = 4-piperidinyl). Data for biol. activity of title compds. were given.

444664-57-7P ΙT RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 1,5-diaryl-7-heterocyclyl(alkyl)-2-quinolinones as p38 protein kinase inhibitors)

RN 444664-57-7 CAPLUS

2(1H) -Quinolinone, 5-(2-chloro-4-fluorophenyl)-1-(2,6-difluorophenyl)-7-CN (triphenylmethyl) - (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 5 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:275968 CAPLUS

DOCUMENT NUMBER: 136:309857

TITLE: Preparation of quinolines and quinolinones as metabotropic glutamate receptor antagonists

INVENTOR(S): Mabire, Dominique Jean-Pierre; Venet, Marc Gaston;

Coupa, Sophie; Poncelet, Alain Philippe; Lesage, Anne

Simone Josephine

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 114 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

WO 2002028837 A1 20020411 WO 2001-EP11135 20010925 < W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,		TENT			KIND DATE		ATE APPLICATION NO.						DATE						
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,																925	<		
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	ΤZ,	UA,	UG,	
			US,	UZ,	VN,	YU,	ZA,	ZW											
		RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	ΑT,	BE,	CH,	CY,	
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BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
CA 2421782 A1 20020411 CA 2001-2421782 20010925 <	CA	2421			•	A 1		2002	0411		CA 2	001-	2421	782				925	<
AU 2001093847 A 20020415 AU 2001-93847 20010925 <	AU	2001	0938	47		А		2002	0415		AU Z	$\cup \cup \bot -$	9384	/			$UU \perp U$	925	<
BR 2001014253 A 20030701 BR 2001-14253 20010925 <	BR	2001	0142	53		А		2003	0701		BR 2	001-	1425	3		2	0010	925	<
EP 1332133 A1 20030806 EP 2001-974298 20010925 <						A1		2003	0806		EP 2	001-	9742	98		2	0010	925	<
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HU 2003002167 A2 20031028 HU 2003-2167 20010925 < JP 2004510764 T 20040408 JP 2002-532423 20010925 < NZ 524945 A 20050128 NZ 2001-524945 20010925	JP	2004	5107	64		Т		2004	0408							2	0010	925	<
JP 2004510764 T 20040408 JP 2002-532423 20010925 < NZ 524945 A 20050128 NZ 2001-524945 20010925	NZ	5249	45			А		2005	0128		NZ 2	0.01 -	5249	45		2	0010	925	
EE 200300126 A 20050415 EE 2003-126 20010925				6		А		2005	0415		EE 2	003-	126			2	0010	925	
CN 1703403 A 20051130 CN 2001-816717 20010925	CN	1703	403																
AII 2001293847 B2 20070524 AII 2001-293847 20010925	AU	2001	2938								ΔΠ 2	001-	2938	47		2	0010	925	
TTD 010065 D1 00000404 TTD 0000 700014 00000011						D 1					KR 2	003-	7020	14		2	0030	211	
HR /UU3UUU//9 AT /UU3UN3U HR /UU3=//9 /UU3U3/4 <==	HR	2003	0002			A1		2003	0630		HK /	いいぅー	//9			/	0030	324	<
IN 2003MN00328 A 20050211 IN 2003-MN328 20030324	IN	2003	0 0 MM	328		A		2005	0211		IN 2	003-	MN32	8		2	0030	324	
BG 107672 A 20040130 BG 2003-107672 20030326 <	BG	1076	72			Α		2004	0130		BG 2	003-	1076	72		2	0030	326	<
ZA 2003002515 A 20040630 ZA 2003-2515 20030331 <	ZA	2003	0025	15		А		2004	0630										
NO 2003001474 A 20030505 NO 2003-1474 20030401 <	NO	2003	0014	74		А					NO 2	003-	1474						
NO 325079 B1 20080128	ИО	3250	79			В1		2008	0128										
MX 2003PA02907 A 20030624 MX 2003-PA2907 20030401 <	MX	2003	PA02	907		А		2003	0624		MX 2	003-	PA29	07		2	0030	401	<
US 20040082592 A1 20040429 US 2003-381987 20030814 <						A1		2004	0429								0030	814	<
US 7115630 B2 20061003	US	7115	630					2006	1003										
US 20050209273 A1 20050922 US 2005-133678 20050520		_		273		A1					US 2	005-	1336	78		2	0050	520	
PRIORITY APPLN. INFO.: EP 2000-203419 A 20001002																			
WO 2001-EP11135 W 20010925		-		•												W 2	0010	925	
US 2003-381987 A3 20030814																A3 2	0030	814	
OTHER SOURCE(S): MARPAT 136:309857	OTHER SO	OURCE	(S):			MARE	PAT	136:	3098										
GI								-	_										

AB The title compds. [I or II; X = O, C(R6)2; (wherein R6 = H, aryl, alkyl, etc.); R1 = alkyl, aryl, thienyl, etc.; R2 = H, halo, CN, etc.; R3, R4 = H, alkyl; or R2 and R3 may be taken together to form (CH2)3, (CH2)4, CH:CHCH:CH, etc.; or R3 and R4 may be taken together to form CH:CHCH:CH, (CH2)4; R5 = H, cycloalkyl, piperidinyl, etc.; Y = O, S; or Y and R5 may be taken together to form CH:NN, N:NN, NCH:CH], useful for treating or preventing glutamate-induced diseases of the central nervous system, were prepared Thus, reacting cis-III [R = C1] with SnMe4 in the presence of Pg(PPh3)4 in PhMe afforded 17% cis-III [R = Me] which showed antagonism at a dose of 2.5 mg/kg bodyweight in cold allodynia test in rats with a Bennett ligation.

IT 409344-47-4P 409344-48-5P 409344-56-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of quinolines and quinolinones as metabotropic glutamate receptor antagonists)

RN 409344-47-4 CAPLUS

CN 2(1H)-Quinolinone, 3-ethyl-6-(2-phenylacetyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2-C & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN 409344-48-5 CAPLUS

CN 2(1H)-Quinolinone, 3-ethyl-6-[2-(2-methoxyphenyl)acetyl]- (CA INDEX NAME)

RN 409344-56-5 CAPLUS

CN 2(1H)-Quinolinone, 3-ethyl-6-(1-oxo-3-phenylpropyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Ph-CH}_2\text{-CH}_2\text{-C} & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:222670 CAPLUS

DOCUMENT NUMBER: 137:241668

TITLE: Phosphonate quinoxalinedione AMPA antagonists for

therapy of stroke and trauma

AUTHOR(S): Ottow, Eckhard; Huth, Andreas; Kruger, Martin;

Schneider, Herbert H.; Neuhaus, Roland; McDonald,

Fiona; Lofberg, Boel; Turski, Lechoslaw

CORPORATE SOURCE: Research Laboratories of Schering AG, Berlin, D-13342,

Germany

SOURCE: Biomedical and Health Research (2001),

45 (Excitatory Amino Acids: Ten Years Later), 329-344

CODEN: BIHREN; ISSN: 0929-6743

PUBLISHER: IOS Press
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:241668

AB Glutamate antagonists derived from the quinoxalinedione scaffold are drug candidates for neuroprotection in stroke and trauma. Quinoxalinedione derivs. such as 2,3-dihydroxy-6-nitro-7-sulfamoylbenzo(f)quinoxaline and 6-(1H-imidazol-1-yl)-7-nitro-2,3-(1H,4H)-quinoxalinedione failed clin. trials because of insoly. and resulting nephrotoxicity. Introduction of phosphonate group into the quinoxalinedione skeleton improves solubility and leaves potency for the α -amino-3-hydroxy-5-methyl-4-isoxazolepropionate (AMPA) receptor unchanged. Phosphonate quinoxalinedione derivs. ZK200775 and ZK202000 protect rodent brain against ischemic and traumatic brain injury. No major deleterious effects on motor coordination, cardiovascular, or respiratory systems are detected in doses required for neuroprotection. No psychotomimetic and no neurotoxic side effects in the brain are observed after treatment with phosphonate quinoxalinediones.

IT 191740-32-6P, ZK202000

RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(phosphonate quinoxalinedione AMPA antagonists for therapy of stroke and trauma)

RN 191740-32-6 CAPLUS

CN Phosphonic acid, [[3,4-dihydro-2,3-dioxo-7-(2-phenylethyl)-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{CH}_2-\operatorname{PO}_3\operatorname{H}_2\\ \\ \operatorname{F}_3\operatorname{C} & \operatorname{N} \\ \\ \operatorname{H} & \operatorname{O} \end{array}$$

IT 191740-18-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(phosphonate quinoxalinedione AMPA antagonists for therapy of stroke and trauma)

RN 191740-18-8 CAPLUS

CN Phosphonic acid, [[3,4-dihydro-2,3-dioxo-7-(2-phenylethyl)-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OEt} \\ \text{CH}_2 & \text{P-OEt} \\ \text{Ph-CH}_2 - \text{CH}_2 & \text{N} & \text{O} \\ \text{F}_3 \text{C} & \text{N} & \text{O} \end{array}$$

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:482884 CAPLUS

DOCUMENT NUMBER: 135:239238

TITLE: A novel quinoline alkaloid possessing a 7-benzyl group

from the centipede, Scolopendra subspinipes

AUTHOR(S): Noda, Naoki; Yashiki, Yuji; Nakatani, Takafumi;

Miyahara, Kazumoto; Du, Xiao-Ming

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Setsunan

University, Osaka, 573-0101, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2001),

49(7), 930-931

CODEN: CPBTAL; ISSN: 0009-2363 Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal LANGUAGE: English

PUBLISHER:

AB The novel quinoline alkaloid scolopendrine was isolated from the centipede, Scolopendra subspinipes mutilans L. Koch. The structure was determined to be 2-hydroxy-7-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-8-quinolyl sulfate on the basis of high-resolution electron-spray ionization mass spectroscopy and two-dimensional NMR spectral data. Unlike quinoline alkaloids so far reported, scolopendrine is unique in having a 7-benzyl moiety in the quinoline ring.

IT 360550-09-0, Scolopendrine

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); RACT (Reactant or reagent)

(quinoline alkaloid from Scolopendra subspinipes)

RN 360550-09-0 CAPLUS

CN 2(1H)-Quinolinone, 7-[(4-hydroxy-3-methoxyphenyl)methyl]-3-methoxy-8-(sulfooxy)- (CA INDEX NAME)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:476381 CAPLUS

DOCUMENT NUMBER: 135:100164

TITLE: $(R)-1-\{(2-0xo-1,2-dihydroquinolin-6-y1)[3-dihydroquinolin-6-y1)[3-dihydroquinolin-6-y1][3-dih$

(trifluoromethyl)phenyl]methyl}-1H-1,2,4-triazol-4-ium

bromide

AUTHOR(S): Peeters, Oswald M.; Blaton, Norbert M.; De Ranter,

Camiel J.

CORPORATE SOURCE: Faculteit Farmaceutische Wetenschappen, Laboratorium

voor Analytische Chemie en Medicinale Fysicochemie, Katholieke Universiteit Leuven, Louvain, B-3000, Belg.

SOURCE: Acta Crystallographica, Section E: Structure Reports

Online (2001), E57(7), o655-o656 CODEN: ACSEBH; ISSN: 1600-5368

URL: http://journals.iucr.org/e/issues/2001/07/00/ya60

33/ya6033.pdf

PUBLISHER: International Union of Crystallography

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB The metabolism of all-trans-retinoic acid is mediated by a cytochrome dependent P 450 system. The title compound, C19H14F3N4O+·Br-(R111214), is an inhibitor of P 450. The three planar ring systems, viz. the triazolyl, Ph and quinolinone groups, are arranged in a propeller-like fashion around the central CH group. The dihedral angles formed by the triazolyl/phenyl, triazolyl/quinolinone and phenyl/quinolinone planes are 55.8(1), 79.85(9) and 78.49(9)°, resp. The N-H...O H bonds, involving the triazolium N-H group and the quinolinone O atom, link the cations into infinite chains stretching along the c axis of the crystal. Crystallog. data are given.

IT 349553-99-7

RL: PRP (Properties)

(crystal structure of)

RN 349553-99-7 CAPLUS

CN 2(1H) -Quinolinone, 6-[(R)-1H-1,2,4-triazol-1-yl[4-

(trifluoromethyl)phenyl]methyl]-, hydrobromide (1:1) (CA INDEX NAME)

Absolute stereochemistry.

● HBr

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:223060 CAPLUS

DOCUMENT NUMBER: 135:5590

TITLE: Some nucleophilic reactions with 6-benzoyl-2,3-

dichloroquinoxaline: synthesis of tetrazolo[1,5-a]quinoxline, 2-methylidene-1,3-dithiolo[4,5-b]quinoxalines, quinoxalino[2,3-b]quinoxalines and pyrazolo[1',5':1,2]imidazolo[4,5-b]-quinoxalines

AUTHOR(S): El-Gaby, M. S. A.; El-Sharief, A. M. Sh; Ammar, Y. A.;

Mohamed, Y. A.; El-Salam, A. A. Abd

CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Al-Azhar

University at Assiut, Assiut, 71524, Egypt

SOURCE: Indian Journal of Chemistry, Section B: Organic

Chemistry Including Medicinal Chemistry (2001

), 40B(3), 195-200

CODEN: IJSBDB; ISSN: 0376-4699

PUBLISHER: National Institute of Science Communication, CSIR

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:5590

AB The starting material 6-benzoyl-2,3-dichloroquinoxaline is subjected to some nucleophilic reagents to study the effect of the benzoyl group on the

reactivity of the two chlorine atoms.

IT 143702-68-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(reactions of 6-benzoyl-2,3-dichloroquinoxaline with nucleophiles)

RN 143702-68-5 CAPLUS

CN 2,3-Quinoxalinedione, 6-benzoyl-1,4-dihydro- (CA INDEX NAME)

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:868071 CAPLUS

DOCUMENT NUMBER: 135:55887

TITLE: Phosphonate quinoxalinedione AMPA antagonists
AUTHOR(S): Turski, Lechoslaw; Schneider, Herbert H.; Neuhaus,
Roland; McDonald, Fiona; Jones, Graham H.; Lofberg,
Boel; Schweinfurth, Hermann; Huth, Andreas; Kruger,

Martin; Ottow, Eckhard

CORPORATE SOURCE: Research Laboratories of Schering AG, Berlin, D-13342,

Germany

SOURCE: Restorative Neurology and Neuroscience (2000

), 17(1), 45-59

CODEN: RNNEEL; ISSN: 0922-6028

PUBLISHER: IOS Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In the Western world, over 350,000 deaths and \$30 billion in medical costs are attributed annually to stroke. Head and spinal cord trauma cause an estimated 250,000 deaths annually and result in medical costs of \$15 billion. Although stroke and head/spinal cord trauma are leading causes of disability and death in humans, no adequate neuroprotective treatment is available. Glutamate antagonists derived from the quinoxalinedione scaffold are as drug candidates for neuroprotection in stroke and trauma. Quinoxalinedione derivs. such as 2,3-dihydroxy-6-nitro-7sulfamoylbenzo(f) quinoxaline and 6-(1H-imidazol-1-yl)-7-nitro-2, 3-(1H, 4H)-1quinoxalinedione failed clin. trials because of insoly. and resulting nephrotoxicity. Introduction of a phosphonate group into the quinoxalinedione skeleton improves solubility and leaves potency for the α -amino-3-hydroxy-5-methyl-4-isoxazolepropionate (AMPA) receptor unchanged. Phosphonate quinoxalinedione derivs. ZK202000 and ZK200775 protected rodent brain against sequelae of permanent occlusion of the middle cerebral artery and head trauma. No major deleterious effects on motor coordination, cardiovascular, or respiratory systems were detected in doses required for neuroprotection. No psychotomimetic and no neurotoxic side effects, typical for N-methyl-D-aspartate antagonists, were observed following treatment with phosphonate quinoxalinediones. ΙT

191740-32-6P, ZK 202000 RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

(phosphonate quinoxalinedione AMPA antagonists as neuroprotectants in stroke and trauma)

RN 191740-32-6 CAPLUS

CN Phosphonic acid, [[3,4-dihydro-2,3-dioxo-7-(2-phenylethyl)-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{CH}_2-\operatorname{PO}_3\operatorname{H}_2\\ \\ \operatorname{Ph}-\operatorname{CH}_2-\operatorname{CH}_2\\ \\ \operatorname{F}_3\operatorname{C} \end{array} \begin{array}{c} \operatorname{CH}_2-\operatorname{PO}_3\operatorname{H}_2\\ \\ \operatorname{N} \\ \operatorname{O} \end{array}$$

REFERENCE COUNT: 69 THERE ARE 69 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:527827 CAPLUS

DOCUMENT NUMBER: 134:162992

TITLE: Synthesis and antimicrobial activities of some novel

quinoxalinone derivatives

AUTHOR(S): Ali, M. M.; Ismail, M. M. F.; El-Gaby, M. S. A.;

Zahran, M. A.; Ammar, Y. A.

CORPORATE SOURCE: Dep. of Chemistry, Faculty of Science, Al-Azhar Univ.,

Cairo, 11884, Egypt

SOURCE: Molecules [online computer file] (2000),

5(6), 864-873

CODEN: MOLEFW; ISSN: 1420-3049

URL: http://www.mdpi.org/molecules/papers/50600864.pdf

PUBLISHER: Molecular Diversity Preservation International

DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:162992

GΙ

AB Condensation of 4-benzoyl-1,2-phenylenediamine with sodium pyruvate in acetic acid furnished two products, which were identified as 6-benzoyl-(I) and 7-benzoyl-3-methyl-2(IH)-quinoxalinone (II). Fusion of I with aromatic aldehydes furnished the styryl derivs. Alkylation of I and II with di-Me sulfate or Et chloroacetate produced the N-alkyl derivs. Hydrazinolysis of one ester derivative with hydrazine hydrate afforded the hydrazide derivative, which underwent condensation with aldehydes to give the corresponding hydrazone derivs. In addition, chlorination of I with thionyl chloride afforded the 2-chloro derivative, which was subjected to reaction with sodium azide and n-butylamine to yield the corresponding tetrazolo (III) and n-butylamino (IV) derivs., resp. The structures of the compds. prepared were confirmed by anal. and spectral data. Also, some of the synthesized compds. were screened for antimicrobial activity.

IT 325469-51-0P 325469-52-1P 325469-58-7P

325469-60-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and antimicrobial activities of quinoxalinone derivs.)

RN 325469-51-0 CAPLUS

CN 2(1H)-Quinoxalinone, 6-benzoyl-3-methyl- (CA INDEX NAME)

RN 325469-52-1 CAPLUS

CN 2(1H)-Quinoxalinone, 7-benzoyl-3-methyl- (CA INDEX NAME)

RN 325469-58-7 CAPLUS

CN 1(2H)-Quinoxalineacetic acid, 6-benzoyl-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 325469-60-1 CAPLUS

CN 1(2H)-Quinoxalineacetic acid, 6-benzoyl-3-methyl-2-oxo-, hydrazide (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

IT 325469-54-3P 325469-59-8P 325469-62-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activities of quinoxalinone derivs.)

RN 325469-54-3 CAPLUS

CN 2(1H)-Quinoxalinone, 6-benzoyl-3-[(1E)-2-(4-methoxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 325469-59-8 CAPLUS

CN 1(2H)-Quinoxalineacetic acid, 7-benzoyl-3-methyl-2-oxo-, ethyl ester (CA INDEX NAME)

RN 325469-62-3 CAPLUS

CN 1(2H)-Quinoxalineacetic acid, 6-benzoyl-3-methyl-2-oxo-, 2-[(4-methoxyphenyl)methylene]hydrazide (CA INDEX NAME)

PAGE 2-A

Double bond geometry as shown.

RN 325469-55-4 CAPLUS CN 2(1H)-Quinoxalinone, 6-benzoyl-3-[(1E)-2-(3,4,5-trimethoxyphenyl)ethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 325469-56-5 CAPLUS

CN 2(1H)-Quinoxalinone, 6-benzoyl-1,3-dimethyl- (CA INDEX NAME)

RN 325469-57-6 CAPLUS

CN 2(1H)-Quinoxalinone, 7-benzoyl-1,3-dimethyl- (CA INDEX NAME)

RN 325469-61-2 CAPLUS

CN 1(2H)-Quinoxalineacetic acid, 6-benzoyl-3-methyl-2-oxo-, 2-(phenylmethylene)hydrazide (CA INDEX NAME)

$$\begin{array}{c} O \\ | \\ | \\ CH_2-C-NH-N \end{array} \\ CH-Ph \\ | \\ O \\ \end{array}$$

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1998:672545 CAPLUS

DOCUMENT NUMBER: 129:275932

ORIGINAL REFERENCE NO.: 129:56265a,56268a

TITLE: Preparation of 3-oxadiazolylquinoxaline derivatives

having affinity to benzodiazepine receptor

INVENTOR(S): Ohno, Kazunori; Odai, Osamu; Furukawa, Kiyoshi; Oka,

Makot

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 43 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO	WO 9842701					A1 19981001				WO 1	998-	JP82	7	19980227 <				
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		DK,	EE,	ES,	FΙ,	GB,	GE,	GH,	GM,	GW,	HU,	ID,	IL,	IS,	JP,	ΚE,	KG,	
		KR,	KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	
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		FR,	GB,	GR,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	
		GΑ,	GN,	ML,	MR,	ΝE,	SN,	TD,	ΤG									
JP	2002	2413	79		Α		2002	0828		JP 1:	997-	8764	6	19970321 <				
AU	9861	179			Α		1998	1020	,	AU 19	998-	6117	9	19980227 <				
PRIORIT						JP 1:	997-	8764	6	1	A 19970321							
						WO 19	998-	JP82	7	W 19980227								

OTHER SOURCE(S): MARPAT 129:275932

GΙ

AB Novel 3-oxadiazolylquinoxaline derivs. represented by general formula (I; wherein Het is oxadiazolyl; R1 is hydrogen, lower alkyl, trifluoromethyl, lower cycloalkyl, lower alkenyl, lower alkynyl, optionally substituted aryl, optionally substituted heteroaryl, or lower alkoxy; R2 is hydrogen, lower alkyl, trifluoromethyl, lower cycloalkyl, halogeno, hydroxy, lower alkoxy, cyano, nitro, acyl, optionally substituted benzoyl, amino, lower mono- or dialkylamino, lower alkoxycarbonylmethyloxy, lower mono- or dialkylaminocarbonylmethyloxy, or optionally substituted benzyloxy; and R3 is hydrogen, lower alkyl, lower cycloalkyl, halogeno, or lower alkoxy), which are useful as a medicine, in particular, which have a selective affinity for benzodiazepine receptors and are useful as a brain activator and a remedy for senile dementia and Alzheimer's disease. Thus, a solution of 1,2-dihydro-2-oxo-3-quinoxalinecarboxylic acid and N,N'-carbonyl diimidazole in DMF was heated with stirring for 3 h at 60° , followed by adding acetamidoxime, and the stirring was continued for another 1.5 h to give 52.6% the title compound (II; R1 = Me; R2 = H). The latter compound and I (R1 = Et, R2 = OMe) inhibited the binding of [3H]diazepam to synaptosome membrane fraction prepared from rat brain with IC50 of 11.5 and 1.41 nM, resp.

IT 213743-73-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxadiazolylquinoxaline derivs. having affinity to benzodiazepine receptor as brain activators and remedies for senile dementia and Alzheimer's disease)

RN 213743-73-8 CAPLUS

CN 2(1H)-Quinoxalinone, 6-benzoyl-3-(3-ethyl-1,2,4-oxadiazol-5-yl)- (CA INDEX NAME)

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:210752 CAPLUS

DOCUMENT NUMBER: 128:257445

ORIGINAL REFERENCE NO.: 128:50967a,50970a

TITLE: Preparation of indolylbenzoquinoxalinones and related

compounds as protein kinase C inhibitors.

INVENTOR(S): Bergstrand, Hakan; Karabelas, Kostas; Sjo, Peter

PATENT ASSIGNEE(S): Astra Aktiebolag (Publ), Swed.

SOURCE: PCT Int. Appl., 63 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	ΓΕΝΤ	NO.			KIN	ND DATE			•	APPL	ICAT	ION :		DATE					
WO	9813		A1 199804			0402		WO 1	 997-		19970919 <								
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		KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,		
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		GN,	ML,	MR,	ΝE,	SN,	TD,	ΤG											
IN	N 1997DE02638				A		2005	0311		IN 1	997-	DE26	38		1	9970	916		
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ZA	9708	469			A		1998	0325		ZA 1	997-								
CA	2265	854			A1		1998	0402		CA 1	997-		19970919 <						
ΑU	9744	:775			A		1998	0417		AU 1	997-	19970919 <							
AU	7162	79			В2		2000	0224											
ΕP	9295	51			A1		1999	0721		EP 1	997-	9432	59		1	9970	919	<	
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US	S 6271231				В1		2001	0807		US 1	997-	9812	66		19971218 <				
US	S 20010025043				A1		2001	0927		US 2	001-	8652	31		20010525 <				

PRIORITY APPLN. INFO.:

SE 1996-3505

SE 1997-2747

WO 1997-SE1582

W 19970919

US 1997-981266

A3 19971218

OTHER SOURCE(S): MARPAT 128:257445

Ι

GΙ

$$\begin{array}{c|c}
O & H & X & Y \\
& & & | & \\
N & & & Z
\end{array}$$

Title compds. [I; A, X, Y, Z = C, N; \geq 2 of A, X, Y, Z = C; may be substituted and/or annulated; excluding 3-(1H-indol-3-yl)-1H-quinoxalin-2-one, 3-(2-methyl-1H-indol-3-yl)-1H-quinoxalin-2-one, and 3-(1,2-diphenyl-1H-indol-3-yl)-1H-quinoxalin-2-one], were prepared as protein kinase C inhibitors (no data). Thus, 1,2-phenylenediamine was stirred overnight with [1-[3-(1,3-dioxoisoindol-2-yl)propyl]-1H-indol-3-yl]oxoacetic acid 2,5-dioxopyrrolidin-1-yl ester (preparation given) in THF to give 3-[3-(3-oxo-3,4-dihydroquinoxalin-2-yl)indol-1-yl]propylammonium acetate. The latter was stirred with MeNH2 in THF/H2O to give 3=[3-(3-oxo-3,4-dihydroquinoxalin-2-yl)indol-1-yl]propylammonium acetate. IT 205377-65-7P 205377-77-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of indolylbenzoquinoxalinones and related compds. as protein kinase C inhibitors)

RN 205377-65-7 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[1-(3-aminopropyl)-1H-indol-3-yl]-1-methyl-6-(phenylmethyl)-, monoacetate (9CI) (CA INDEX NAME)

CM 1

CRN 205377-64-6 CMF C27 H26 N4 O

CM 2

CRN 64-19-7

RN 205377-77-1 CAPLUS

CN 2(1H)-Quinoxalinone, 3-[1-(3-aminopropyl)-1H-indol-3-yl]-6-(phenylmethyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 205377-76-0 CMF C26 H24 N4 O

CM 2

CRN 76-05-1 CMF C2 H F3 O2

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:447997 CAPLUS

DOCUMENT NUMBER: 127:81611
ORIGINAL REFERENCE NO.: 127:15657a

TITLE: Preparation of novel quinoxalinedione derivatives as

medicaments

INVENTOR(S): Huth, Andreas; Krueger, Martin; Ottow, Eckhard;

Seidelmann, Dieter; Neuhaus, Roland; Schneider,

Herbert; Turski, Lechoslaw

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 9 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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                                19970528
                                            DE 1995-19545251
                                                                   19951124 <--
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                                                                   19961115 <--
                          Α1
                                19970529
                                            CA 1996-2238023
                                19970529
                                            WO 1996-DE2227
     WO 9719066
                         Α1
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     AU 9718674
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                                            NO 1998-2349
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                          Α
                                19980701
PRIORITY APPLN. INFO.:
                                            DE 1995-19545251
                                                                A 19951124
                                            WO 1996-DE2227
                                                                W 19961115
OTHER SOURCE(S):
                        MARPAT 127:81611
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Ι

INDEX NAME)

GΙ

AB The preparation of title compds. I (R1 = phosphonyl, sulfonyl, or carboxy substituted organo, cyanoorgano, tetrazolylorgano, etc.; R5 = substituted amino, thionyl, carbonyl, etc.; R6, R7 = same or different H, halo, NO2, cyano, substituted amino, carbonyl, alkoxy, hetaryl, etc.), useful as medicaments for central nerves system, is described. Thus, [(6-trifluoromethyl-7-[N-oxy-(N-isopropylformylimino)]-1,2,3,4tetrahydroquinoxalin-2,3-dion)-1-yl]methanephosphonic acid was prepared in several steps starting from aminomethanephosphonic acid. 191740-18-8P 191740-19-9P 191740-20-2P ΙT 191740-21-3P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of novel quinoxalinedione derivs. as medicaments) 191740-18-8 CAPLUS RN Phosphonic acid, [[3,4-dihydro-2,3-dioxo-7-(2-phenylethyl)-6-CN (trifluoromethyl)-1(2H)-quinoxalinyl]methyl]-, diethyl ester (9CI) (CA

$$\begin{array}{c|c} \text{OEt} \\ \text{CH}_2 & \text{P-OEt} \\ \text{Ph-CH}_2 - \text{CH}_2 & \text{N} & \text{O} \\ \text{F}_3 \text{C} & \text{N} & \text{O} \end{array}$$

RN 191740-19-9 CAPLUS

CN Phosphonic acid, [[7-[2-(4-chlorophenyl)ethyl]-3,4-dihydro-2,3-dioxo-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2 & \text{OEt} \\ \text{CH}_2 & \text{P-OEt} \\ \text{NOOO} \\ \text{F}_3\text{C} & \text{NOOO} \\ \end{array}$$

RN 191740-20-2 CAPLUS

CN Phosphonic acid, [[7-[2-(4-fluorophenyl)ethyl]-3,4-dihydro-2,3-dioxo-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OEt} \\ & \text{CH}_2 & \text{P-OEt} \\ & \text{N} & \text{O} \\ & \text{F}_3\text{C} & \text{N} & \text{O} \end{array}$$

RN 191740-21-3 CAPLUS

CN Phosphonic acid, [[3,4-dihydro-7-[2-(4-methoxyphenyl)ethyl]-2,3-dioxo-6-(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]-, diethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OEt} \\ & \text{CH}_2 \\ & \text{P-OEt} \\ & \text{N} \\ & \text{O} \end{array}$$

IT 191740-32-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of novel quinoxalinedione derivs. as medicaments)

RN 191740-32-6 CAPLUS

CN Phosphonic acid, [[3,4-dihydro-2,3-dioxo-7-(2-phenylethyl)-6-

(trifluoromethyl)-1(2H)-quinoxalinyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{CH}_2-\operatorname{PO}_3\operatorname{H}_2 \\ \\ \operatorname{Ph-CH}_2-\operatorname{CH}_2 \\ \\ \operatorname{F}_3\operatorname{C} \\ \end{array}$$

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:527663 CAPLUS

DOCUMENT NUMBER: 125:167994

ORIGINAL REFERENCE NO.: 125:31485a,31488a

TITLE: Preparation of 6-[triazolyl(3-

trifluoromethylphenyl)methyl]-2-quinolin(thi)ones for

treatment of keratinization disorders

INVENTOR(S): Venet, Marc Gaston; Mabire, Dominique Jean-Pierre;

Sanz, Gerard Charles

PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.

SOURCE: PCT Int. Appl., 32 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE			APPLICATION NO.					DATE						
WO 9620200				A1 19960704		,	WO 1995-EP5173				19951221 <							
	W:	AL,	AM,	AU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	FI,	GE,	HU,	IS,	JP,	,
		KE,	KG,	KP,	KR,	KΖ,	LK,	LR,	LS,	LT,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	,
					RO,													
	RW:	KE,																
					ΝL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML ,	MR,	,
				TD,														
IN 1995CA01685								IN 1995-CA1685										
	CA 2207268				19960704			CA 1995-2207268										
	AU 9644362										1	9951	221	<				
	AU 698199				1998			EP 1995-943237										
	EP 800524					1015		EP 1	995-	9432.	37		1	9951	221	<		
EP	8005				В1		2001											
		AT,	BE,	CH,		,												
	1171				A			0128	1	CN 1	995-	1971	62		1	9951	221	<
	1085				В		2002			4	005		0.0			0054	004	
	1051				Τ		1998				995-					9951		
	9510				A		1999	–			995-					9951		
RU	2165				C2		20010420			RU 1997-112898				9951				
	2079				Τ		20011115			AT 1995-943237				9951				
	8005				T		20020429			PT 1995-943237				9951				
_	2166				T3		20020501			ES 1995-943237 PL 1995-321041								
	1829				B1			0531										
ZΑ	9510	989			А		199/	0627		ZA I	995-	T088.	9		1	9951	221	<

IL 116577	A	20000229	IL	1995-116577		19951227 <
US 5922734	A	19990713	US	1997-860239		19970616 <
FI 9702794	A	19970627	FI	1997-2794		19970627 <
NO 9703029	А	19970627	NO	1997-3029		19970627 <
NO 311220	B1	20011029				
PRIORITY APPLN. INFO.:			ΕP	1994-203773	A	19941228
			WO	1995-EP5173	W	19951221
OTHER COHREE(C).	MADDAT	125.16700/				

OTHER SOURCE(S): MARPAT 125:167994

AB Title compds. [I; R = 3-(F3C)C6H4][II; R1 = H, NH2, alkyl; R2,R3 = H, halo, alkyl; X = O or S; 1 of Z1,Z2 = N and the other = CH] were prepared Thus, (R)-II (R1-R3 = H, X = O, Z1 = N, Z2 = CH) gave complete suppression of estradiol undecylate-induced vaginal keratinization in 50% of ovariectomized rats at 1.25mg/kg orally

ovariectomized rats at 1.25mg/kg orally.

180421-65-2P 180421-66-3P 180421-67-4P 180421-68-5P 180421-69-6P 180421-70-9P 180421-71-0P 180421-72-1P 180421-73-2P 180421-74-3P 180421-75-4P 180421-76-5P 180421-77-6P 180421-78-7P 180421-79-8P 180421-80-1P 180421-81-2P 180421-82-3P 180421-83-4P 180421-85-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 6-[triazolyl(3-trifluoromethylphenyl)methyl]-2quinolin(thi)ones for treatment of keratinization disorders)

RN 180421-65-2 CAPLUS

CN 2(1H)-Quinolinone, 6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]-, (R)- (9CI) (CA INDEX NAME)

Ι

Absolute stereochemistry. Rotation (-).

RN 180421-66-3 CAPLUS
CN 2(1H)-Quinolinone, 6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 180421-67-4 CAPLUS CN 2(1H)-Quinolinone, 6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-68-5 CAPLUS
CN 2(1H)-Quinolinone, 6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)

RN 180421-69-6 CAPLUS
CN 2(1H)-Quinolinone, 6-[fluoro-1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-70-9 CAPLUS

CN 2(1H)-Quinolinone, 6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]propyl]- (CA INDEX NAME)

RN 180421-71-0 CAPLUS

CN 2(1H)-Quinolinone, 6-[2-methyl-1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]propyl]- (CA INDEX NAME)

RN 180421-72-1 CAPLUS

CN 2(1H)-Quinolinone, 6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]pentyl]- (CA INDEX NAME)

RN 180421-73-2 CAPLUS

CN 2(1H)-Quinolinone, 8-methyl-6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-74-3 CAPLUS

CN 2(1H)-Quinolinone, 5-chloro-6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-75-4 CAPLUS

CN 2(1H)-Quinolinone, 8-fluoro-6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-76-5 CAPLUS

CN 2(1H)-Quinolinone, 1-fluoro-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)

RN 180421-77-6 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)

RN 180421-78-7 CAPLUS

CN 2(1H)-Quinolinone, 1-ethyl-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)

RN 180421-79-8 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]propyl]- (CA INDEX NAME)

RN 180421-80-1 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]butyl]- (CA INDEX NAME)

RN 180421-81-2 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]pentyl]- (CA INDEX NAME)

RN 180421-82-3 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[3-methyl-1-(1H-1,2,4-triazol-1-yl)-1-[3-(trifluoromethyl)phenyl]butyl]- (CA INDEX NAME)

RN 180421-83-4 CAPLUS

CN 2(1H)-Quinolinone, 1-amino-6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]- (CA INDEX NAME)

RN 180421-85-6 CAPLUS

CN 2(1H)-Quinolinone, 1-methyl-6-[1H-1,2,4-triazol-1-yl[3-(trifluoromethyl)phenyl]methyl]-, monohydrobromide, (R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

• HBr

L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:217224 CAPLUS

DOCUMENT NUMBER: 120:217224

ORIGINAL REFERENCE NO.: 120:38557a,38560a

TITLE: Studies of 1-alkyl-2(1H)-pyridone derivatives. XXXV.

The Friedel-Crafts reaction of 1-methyl-2(1H)-pyridone

homologs with benzoic acid derivatives

AUTHOR(S): Fujita, Reiko; Yasugahira, Hiroaki; Tomisawa, Hiroshi

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, 981, Japan

SOURCE: Annual Report of the Tohoku College of Pharmacy (

1992), 39, 91-9

CODEN: TYKNAQ; ISSN: 0495-7342

DOCUMENT TYPE: Journal LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 120:217224

AB The Friedel-Crafts reaction of 1-methyl-2(1H)-quinolone with o-bromobenzoyl chloride (I) gave 6-(o-bromobenzoyl)-1-methyl-2(1H)-quinolone in good yield. The reaction of 1,4-dimethyl-2(1H)-quinolone, 4-benzoyl-1-methyl-2(1H)-quinolone, or 2,3-dimethyl-1(2H)-isoquinolone with BzCl or Bz2O gave regioselectively 6-benzoyl-1,4-dimethyl-2(1H)-

quinolone, 4,6-dibenzoyl-1-methyl-2(1H)-quinolone, or 4-benzoyl-2,3-dimethyl-1(2H)-isoquinolone, resp. The reaction of 2,6,7-trimethyl-1(2H)-

isoquinolone with I gave 5-(o-bromobenzoy1)-2,6,7-trimethyl-1(2H)-

isoquinolone.

RN 153888-51-8 CAPLUS

CN 2(1H)-Quinolinone, 6-(2-bromobenzoyl)-1-methyl- (CA INDEX NAME)

L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:592207 CAPLUS

DOCUMENT NUMBER: 117:192207

ORIGINAL REFERENCE NO.: 117:33223a,33226a

TITLE: Fluorine-19 NMR studies on the mechanism of riboflavin synthase. Synthesis of 6-(trifluoromethyl)-7-oxo-8-(D-

ribityl) lumazine and 6-(trifluoromethyl)-7-methyl-8-(D-

ribityl) lumazine

AUTHOR(S): Cushman, Mark; Patel, Hemantkumar H.; Scheuring,

Johannes; Bacher, Adelbert

CORPORATE SOURCE: Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette,

IN, 47907, USA

SOURCE: Journal of Organic Chemistry (1992), 57(21),

5630 - 43

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title oxo-(D-ribityl)lumazine I was synthesized by reaction of Me trifluoropyruvate with 5-amino-6-(D-ribitylamino)pyrimidine-2,4(1H,3H)-dione hydrochloride and utilized as a 19F NMR probe of the light riboflavin synthase of Bacillus subtillis. I was found to be an inhibitor of riboflavin synthase with an inhibition constant KI = 55 μM . The

enzyme-bound ligand gave rise to several broad 19F NMR signals which were shifted to low field. The bound ligand I could be displaced from the enzyme by the enzyme product, riboflavin (II), and the product analog, 5-nitroso-6-(ribitylamino)-2,4(1H,3H)-pyrimidinedione. Title methyl-(D-ribityl)lumazine III was synthesized by reaction of 5-amino-6-(D-ribitylamino)pyrimidine-2,4(1H,3H)-dione hydrochloride with 1,1,1-trifluorobutane-2,3-dione. Three mols. of III can be bound relatively tightly per mol of riboflavin synthase, i.e., one ligand mol. per protein subunit. A scheme for the catalytic cycle of riboflavin synthase is proposed.

143309-79-9P 143309-80-2P ΙT

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 143309-79-9 CAPLUS

2(1H)-Quinoxalinone, 6-benzoyl-3-(trifluoromethyl)- (CA INDEX NAME) CN

143309-80-2 CAPLUS

CN 2(1H)-Quinoxalinone, 7-benzoyl-3-(trifluoromethyl)- (CA INDEX NAME)

ANSWER 18 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

1992:571381 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 117:171381

ORIGINAL REFERENCE NO.: 117:29633a,29636a

Synthesis of pyrido[1',2':1,2]imidazo[4,5-TITLE:

b]quinoxalines

Tanaka, Kiyoshi; Takahashi, Hideki; Takimoto, Kozo; AUTHOR(S):

Sugita, Masahiko; Mitsuhashi, Keiryo

Fac. Eng., Seikei Univ., Musahino, 180, Japan CORPORATE SOURCE:

Journal of Heterocyclic Chemistry (1992), SOURCE:

29(4), 771-7 CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 117:171381

GΙ

AB Synthesis of title compds. I (R = H, 8-, 9-Cl, 8-, 9-Bz, 8-, 9-NO2; R1 = H, 1-, 2-, 3-, 4-Me, 4-PhCH2O) by the facile cyclizations of 2,3-dichloroquinoxalines II with 2-aminopyridines III and of 2-amino-3-chloroquinoxalines IV (R \neq H) with various substituted pyridines is described.

IT 143702-68-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (chlorination of)

RN 143702-68-5 CAPLUS

CN 2,3-Quinoxalinedione, 6-benzoyl-1,4-dihydro- (CA INDEX NAME)

$$\begin{array}{c|c} O & H & O \\ H & N & O \\ \hline & N & O \\ \end{array}$$

L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:612014 CAPLUS

DOCUMENT NUMBER: 113:212014

ORIGINAL REFERENCE NO.: 113:35835a,35838a

TITLE: Preparation of (1H-azol-1-ylmethyl)quinolines,

-quinazolines, and -quinoxalines as drugs

INVENTOR(S): Freyne, Eddy Jean Edgard; Venet, Marc Gaston;

Raeymaekers, Alfons Herman Margaretha; Sanz, Gerard

Charles

PATENT ASSIGNEE(S): Janssen Pharmaceutica N. V., Belg.

SOURCE: Eur. Pat. Appl., 106 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 371564	A2	19900606	EP 1989-203014	19891128 <	
EP 371564	A3	19910529			
EP 371564	B1	19950712			
R: AT, BE, CH,	DE, ES	, FR, GB,	GR, IT, LI, LU, NL, SE		
US 5028606	A	19910702	US 1989-434957	19891113 <	
US 5037829	A	19910806	US 1989-435120	19891113 <	
CA 2002864	A1	19900529	CA 1989-2002864	19891114 <	
CA 2002864	С	19991116			

	8905994	A	19900530	DK	1989-5994		19891128	<		
	172748	B1	19990628							
	8904734	A	19900530	ИО	1989-4734		19891128	<		
	174509	В	19940207							
NO	174509	С	19940518							
AU	8945646	A	19900607	ΑU	1989-45646		19891128	<		
AU	620946	B2	19920227							
HU	52498	A2	19900728	HU	1989-6220		19891128	<		
HU	205106	В	19920330							
ZA	8909076	A	19910731	ZA	1989-9076		19891128	<		
SU	1780536	A3	19921207	SU	1989-4742543		19891128	<		
$_{ m IL}$	92486	A	19930708	IL	1989-92486		19891128	<		
ES	2088889	Т3	19961001	ES	1989-203014		19891128	<		
FI	101964	В	19980930	FI	1989-5687		19891128	<		
FI	101964	В1	19980930							
CN	1042912	A	19900613	CN	1989-108925		19891129	<		
CN	1033752	В	19970108							
JP	02223579	A	19900905	JΡ	1989-307793		19891129	<		
JP	2916181	В2	19990705							
US	5151421	A	19920929	US	1991-672298		19910320	<		
US	5185346	A	19930209	US	1991-704746		19910523	<		
US	5268380	A	19931207	US	1992-973871		19921110	<		
US	5441954	A	19950815	US	1993-131817		19931005	<		
CN	1106004	A	19950802	CN	1994-117801		19941102	<		
CN	1036002	В	19971001							
CN	1106005	A	19950802	CN	1994-117802		19941102	<		
CN	1036003	В	19971001							
US	5612354	A	19970318	US	1995-409551		19950323	<		
PRIORIT:	Y APPLN. INFO.:			GB	1988-27820	Α	19881129			
				GB	1988-27821	Α	19881129			
				GB	1988-27822	Α	19881129			
				US	1989-434205	В2	19891113			
				US	1989-434957	АЗ	19891113			
					1991-704746		19910523			
					1992-973871		19921110			
					1993-131817		19931005			
OTHER SOURCE(S): MARPAT 113:212014										
		-								

The title compds. [I; R = H, alkyl; X1:X2 = CH:CH, CH:N, N:CH; Y = H, AΒ alkyl, cycloalkyl, alkenyl, alkynyl, (un)substituted aryl, aralkyl; Z = (un) substituted (oxo) quinolinyl, (oxo- or thioxo) quinazolinyl, (oxo- or dioxo)quinoxalinyl] were prepared as retinoic acid metabolism inhibitors, aromatase inhibitors, etc. Thus, 3,4-dihydroquinolin-2(1H)-one was stirred 2 h at 70° with BzCl in DMF containing AlCl3 and the product reduced by NaBH4 to give hydroxymethylquinolinone II (R1 = Ph, R2 = OH). II (R1 = Me, R2 = OH) was stirred overnight with SOC12 in THF and the product II (R1 = Me, R2 = C1) stirred overnight at $60-70^{\circ}$ with 1H-imidazole in DMSO to give II (R1 = Me, R2 = imidazolo) which maintained plasma levels of i.v. administered all-trans-retinoic acid at ≥ 10 ng/mL in rats 2 h after oral administration of 40 mg/kg.

120067-41-6P 130344-00-2P 130344-01-3P 130344-02-4P 130344-03-5P 130346-18-8P 130346-22-4P 130346-25-7P 130346-26-8P 130346-27-9P 130346-30-4P 130346-32-6P 130346-33-7P 130346-36-0P 130346-38-2P 130346-40-6P 130346-41-7P 130346-42-8P 130346-50-8P 130346-51-9P 130346-66-6P 130346-67-7P 130346-68-8P 130346-69-9P 130346-70-2P 130346-74-6P 130346-78-0P 130347-21-6P 130347-22-7P 130347-23-8P 130347-24-9P 130347-25-0P 130347-26-1P 130347-27-2P 130347-28-3P 130347-29-4P 130347-30-7P 130347-31-8P 130347-33-0P 130347-35-2P 130347-37-4P 130347-38-5P 130347-39-6P 130347-40-9P 130347-41-0P 130347-42-1P 130347-44-3P 130347-45-4P 130347-62-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as retinoate metabolism and aromatase inhibitor) RN 120067-41-6 CAPLUS CN 2(1H)-Quinolinone, 6-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & H \\ & & & \\ N & & CH \end{array}$$

RN 130344-00-2 CAPLUS CN 2(1H)-Quinolinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130344-01-3 CAPLUS CN 2(1H)-Quinolinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130344-02-4 CAPLUS CN 2(1H)-Quinolinone, 6-[(3-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130344-03-5 CAPLUS

CN 2(1H)-Quinolinone, 6-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130346-18-8 CAPLUS

CN 2(1H) -Quinoxalinone, 6-(1H-imidazol-1-ylphenylmethyl)-3-methyl- (CA INDEX NAME)

RN 130346-22-4 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[1H-imidazol-1-yl[3-(trifluoromethyl)phenyl]methyl]-3-methyl- (CA INDEX NAME)

RN 130346-25-7 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(2-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-26-8 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-

(CA INDEX NAME)

$$\begin{array}{c|c} & N \\ & N \\ & N \\ & CH \\ & N \\ & N \\ & H \\ & O \\ \end{array}$$

RN 130346-27-9 CAPLUS
CN 2(1H)-Quinoxalinone, 6-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl(CA INDEX NAME)

$$\begin{array}{c|c} N \\ N \\ CH \\ N \\ N \\ N \\ N \\ O \end{array}$$

RN 130346-30-4 CAPLUS CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-32-6 CAPLUS
CN 2(1H)-Quinoxalinone, 1-butyl-6-(1H-imidazol-1-ylphenylmethyl)-3-methyl(CA INDEX NAME)

RN 130346-33-7 CAPLUS

RN 130346-36-0 CAPLUS CN 2(1H)-Quinoxalinone, 7-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-38-2 CAPLUS CN 2(1H)-Quinoxalinone, 7-[(3-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-40-6 CAPLUS
CN 2(1H)-Quinoxalinone, 7-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 130346-39-3 CMF C19 H15 F N4 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 130346-41-7 CAPLUS

CN 2(1H)-Quinoxalinone, 1-amino-6-(1H-imidazol-1-ylphenylmethyl)-3-methyl-(CA INDEX NAME)

RN 130346-42-8 CAPLUS

CN 2(1H)-Quinoxalinone, 6-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

RN 130346-50-8 CAPLUS

CN 2(1H)-Quinoxalinone, 7-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

RN 130346-51-9 CAPLUS

CN 2(1H)-Quinoxalinone, 6-(1H-imidazol-1-ylphenylmethyl)-3-phenyl- (CA INDEX NAME)

RN 130346-66-6 CAPLUS CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-67-7 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-methyl-(CA INDEX NAME)

RN 130346-68-8 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(1H-imidazol-1-yl)(4-methoxyphenyl)methyl]-3-methyl- (9CI) (CA INDEX NAME)

RN 130346-69-9 CAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-6-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

RN 130346-70-2 CAPLUS

CN 2(1H)-Quinoxalinone, 3-ethyl-7-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{H} & \text{O} \\ & & \text{CH} & \text{N} & \text{O} \\ \end{array}$$

RN 130346-74-6 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl(4-methylphenyl)methyl]-3-methyl-(CA INDEX NAME)

RN 130346-78-0 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl(4-methoxyphenyl)methyl]-3-methyl-(CA INDEX NAME)

RN 130347-21-6 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-phenyl-, 4-oxide (CA INDEX NAME)

RN 130347-22-7 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-phenyl-(CA INDEX NAME)

RN 130347-23-8 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[1H-imidazol-1-yl[4-(1-methylethyl)phenyl]methyl]-3-methyl- (CA INDEX NAME)

RN 130347-24-9 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[1H-imidazol-1-yl[4-(1-methylethyl)phenyl]methyl]-3-methyl- (CA INDEX NAME)

RN 130347-25-0 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-, 4-oxide (CA INDEX NAME)

RN 130347-26-1 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130347-27-2 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(2-methylpropyl)- (CA INDEX NAME)

RN 130347-28-3 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(2-methylpropyl)- (CA INDEX NAME)

RN 130347-29-4 CAPLUS

 $\texttt{CN} \qquad \texttt{2(1H)-Quinoxalinone, 7-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl-1}$

RN 130347-30-7 CAPLUS CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl-(CA INDEX NAME)

RN 130347-31-8 CAPLUS
CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(1-methylethyl)- (CA INDEX NAME)

RN 130347-33-0 CAPLUS CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130347-35-2 CAPLUS

RN 130347-37-4 CAPLUS CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl-(CA INDEX NAME)

RN 130347-38-5 CAPLUS
CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-propyl(CA INDEX NAME)

RN 130347-39-6 CAPLUS
CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(1-methylpropyl)- (CA INDEX NAME)

RN 130347-40-9 CAPLUS

CN 2(1H)-Quinoxalinone, 7-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(1-methylpropyl)- (CA INDEX NAME)

RN 130347-41-0 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(4-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-(1-methylethyl)- (CA INDEX NAME)

RN 130347-42-1 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3-chlorophenyl)-1H-imidazol-1-ylmethyl]-3-phenyl-(CA INDEX NAME)

RN 130347-44-3 CAPLUS

CN 2(1H)-Quinoxalinone, 3-benzoyl-6-(1H-imidazol-1-ylphenylmethyl)-, 4-oxide (CA INDEX NAME)

RN 130347-45-4 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(4-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130347-46-5 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(2-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130347-47-6 CAPLUS

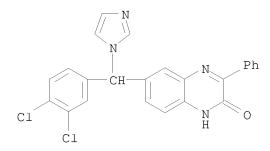
CN 2(1H)-Quinoxalinone, 6-[(3-fluorophenyl)-1H-imidazol-1-ylmethyl]- (CA INDEX NAME)

RN 130347-48-7 CAPLUS

CN 2(1H)-Quinoxalinone, 3-phenyl-6-(phenyl-1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 130347-62-5 CAPLUS

CN 2(1H)-Quinoxalinone, 6-[(3,4-dichlorophenyl)-1H-imidazol-1-ylmethyl]-3-phenyl- (CA INDEX NAME)



L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:552215 CAPLUS

DOCUMENT NUMBER: 113:152215

ORIGINAL REFERENCE NO.: 113:25867a,25870a

TITLE: Studies on 1-alkyl-2(1H)-pyridone derivatives. XXXII.

The Friedel-Crafts reaction of 1-alkyl-2(1H)-pyridone

derivatives with acid anhydride Fujita, Reiko; Tomisawa, Hiroshi

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, 981, Japan SOURCE: Yakugaku Zasshi (1990), 110(6), 449-52

CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 113:152215

AB Reaction of N-benzyl- (I) and N-phenethyl-2(1H)-pyridone (II) with Bz20 (III) gave 5-benzoyl and 3,5-dibenzoyl compds. in good yields. Reactions of I and II with Ac20 gave only 5-acetyl compds. Reactions of dimethyl-2(1H)-pyridione bearing one Me group on the pyridone ring with III were carried out. Only 1,3-dimethyl-2(1H)-pyridone gave the 5-benzoyl-1,3-dimethyl compound; the others gave no benzoyl compound Reactions with Ac20 gave either a 5-acetyl compound or no acetyl compound Reactions of thiolactam compds. (thiopyridone, thioquinolone) with III gave 5-benzoylpyridone and 6-benzoylquinone in poor yields, resp.

IT 53995-93-0P

AUTHOR(S):

RN 53995-93-0 CAPLUS

CN 2(1H)-Quinolinone, 6-benzoyl-1-methyl- (CA INDEX NAME)

Ph-C

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1989:407401 CAPLUS

DOCUMENT NUMBER: 111:7401

ORIGINAL REFERENCE NO.: 111:1422h,1423a

TITLE: Imidazole- or pyridine-containing carbostyrils as

combined thromboxane synthetase and cyclic-AMP phosphodiesterase inhibitors, their preparation, and

pharmaceuticals containing them

INVENTOR(S): Walker, Keith A. M.; Bruno, John J.; Martinez, Gregory

R.

PATENT ASSIGNEE(S): Syntex (U.S.A.), Inc., USA

Ι

SOURCE: U.S., 20 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
		1.0001.000			10060500
US 4792561	A	19881220	US 1986-868845		19860529 <
US 4921862	A	19900501	US 1988-247134		19880921 <
PRIORITY APPLN. INFO.:			US 1986-868845	А3	19860529
OTHER SOURCE(S):	CASREA	CT 111:7401;	MARPAT 111:7401		
GI					

Title compds. I [X = R1CR2, cis- or trans-CR3:CR4; R1 = H when R2 = OH, or R1 = Ph, phenylalkyl when R2 = H, OH; Ph is optionally monosubstituted; or R1R2 = O, C1-6 alkylidene, (substituted) benzylidene; R3 = H, C1-6 alkyl; R4 = H; R3R4 = bond; n = 0-3; R = 1-imidazolyl; dotted line = optional covalent bond] are prepared as thromboxane synthetase and cAMP phosphodiesterase inhibitors for treatment of disease characterized by elevated thromboxane levels or an imbalance of prostacyclin/thromboxane levels (no data). A mixture of CuI 11.6, (Ph3P)2PdC12 86, N-propargylimidazole (preparation given) 774 mg, and 6-bromo-3,4-dihydrocarbostyril 1.5 g was stirred in 10mL pyridine and 2 mL triethylamine at 100° for 48 h under N. The reaction mixture was then treated with saturated aqueous K2CO3, extracted with 10% MeOH in CH2C12,

worked up to give 6-[3-(imidazol-1-yl)-1-propyn-1-yl]-3,4-dihydrocarbostyril. The latter (502 mg) was stirred under H in the presence of 200 mg 10% Pd/C to give 6-[3-(imidazol-1-yl)propyl]-3,4-dihydrocarbostyril (II). A tablet was formulated containing II 25, cornstarch 20, spray-dried lactose 153, and Mg stearate 2 mg.

IT 120067-41-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as cAMP phosphodiesterase and thromboxane synthetase inhibitors)

RN 120067-41-6 CAPLUS

CN 2(1H)-Quinolinone, 6-(1H-imidazol-1-ylphenylmethyl)- (CA INDEX NAME)

L4 ANSWER 22 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1988:610869 CAPLUS

DOCUMENT NUMBER: 109:210869

ORIGINAL REFERENCE NO.: 109:34879a,34882a

TITLE: Carbinolamine equivalents in the 8-

aminotetrahydroisoquinoline series

AUTHOR(S): Moehrle, Hans; Biegholdt, Martin

CORPORATE SOURCE: Inst. Pharm. Chem., Univ. Duesseldorf, Duesseldorf,

4000/1, Fed. Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1988

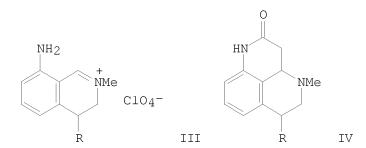
), 321(5), 287-91

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 109:210869

GI



AB Hg(II)-EDTA dehydrogenations of the tetrahydroisoquinolines I (R = H, Ph) do not yield the expected pure carbinolamines, but the dimers II in an intermol. reaction. The acetylation of the dimers or of the iminium salts III generates the tricyclic primary products IV which undergo cleavage when the reaction time is prolonged.

IT 117366-00-4P

RN 117366-00-4 CAPLUS

CN Acetamide, N-[2-(1,2-dihydro-2-oxo-5-quinolinyl)-2-phenylethyl]-N-methyl-

L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:153494 CAPLUS

DOCUMENT NUMBER: 90:153494

ORIGINAL REFERENCE NO.: 90:24415a,24418a TITLE: Fluorescent dyes

INVENTOR(S): Eckstein, Udo; Theidel, Hans PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 41 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2730644 EP 346 EP 346	A1 A1 B1	19790125 19790124 19800109	DE 1977-2730644 EP 1978-100253	19770707 < 19780628 <
R: CH, DE, FR, JP 54017933		19790209	JP 1978-81040	19780705 <
US 4184977 PRIORITY APPLN. INFO.: GI	А	19800122	US 1978-922186 DE 1977-2730644	19780705 < 19770707

$$\begin{array}{c|c} R & N \\ R1 & N \end{array} \qquad \begin{array}{c} CH = CH \\ \end{array} \qquad \begin{array}{c} R2 \\ \end{array} \qquad \begin{array}{c} R \\$$

AB Fluorescent quinoxalines of general structure I were prepared, where R and R1 = H, halogen, alkyl, alkenyl, OH, alkoxy, aryloxy, amino, or substituted amino, R2 = H or an aryl or heterocyclic group, and n = 0, 1, or 2. I are especially useful as fluorescent whiteners. Thus, condensation of 2-(4-formylphenyl)benzoxazole [27395-93-3] with 2,3-dimethoxy-6- (dimethoxyphosphonomethyl)quinoxaline [69722-49-2] in DMF to which NaOMe was added portionwise gave I [R = R1 = MeO, n = 1, R2 = 2-benzoxazolyl (para position)] [69722-71-0], which showed a reddish blue fluorescence when dissolved in DMF and a fast, strong whitening effect in poly(ethylene terephthalate). Other I were similarly prepared

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and reaction with thionyl chloride)

RN 69722-55-0 CAPLUS

CN 2,3-Quinoxalinedione, 6-[2-[4-(2-benzoxazoly1)pheny1]etheny1]-1,4-dihydro-(CA INDEX NAME)

L4 ANSWER 24 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:443155 CAPLUS

DOCUMENT NUMBER: 83:43155

ORIGINAL REFERENCE NO.: 83:6819a,6822a

TITLE: 1-Alky1-2(1H)-pyridone derivatives. XXIV.

Friedel-Crafts reaction of 1-methyl-2(1H)-pyridone and

its derivatives with acid anhydride

AUTHOR(S): Tomisawa, Hiroshi; Fujita, Reiko; Hongo, Hiroshi;

Kato, Hideki

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1975),

23(3), 592-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English

AB The Friedel-Crafts reactions of 1-methyl-2(1H)-pyridone (I),

2-methyl-1(2H)-isoquinolone (II), and 1-methyl-2(1H)-quinolone (III) with acid anhydrides, principally Bz2O, were carried out. In the case of I and II, reaction with acid anhydride gave the products in a good yield, but in the case of III, the reaction with acid anhydride gave products in much less yield than that with acid chloride.

IT 53995-93-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 53995-93-0 CAPLUS

CN 2(1H)-Quinolinone, 6-benzoyl-1-methyl- (CA INDEX NAME)

L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1974:551956 CAPLUS

DOCUMENT NUMBER: 81:151956

ORIGINAL REFERENCE NO.: 81:23681a,23684a

TITLE: 1-Alkyl-2(1H)-pyridone derivatives. XXII.

Friedel-Crafts reaction of 1-methyl-2(1H)-pyridone and

its homologs with benzoyl chloride

AUTHOR(S): Tomisawa, Hiroshi; Fujita, Reiko; Hongo, Hiroshi;

Kato, Hideki

CORPORATE SOURCE: Tohoku Coll. Pharm., Sendai, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1974),

22(9), 2091-6

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English

AB Friedel-Crafts reaction of 1-methyl-2(1H)-pyridone, 1-methyl-2(1H)-

quinolone, and 2-methyl-1 (2H)-isoquinolone with BzCl gave

5-benzoyl-1-methyl-2(1H)-pyridone, 3-benzoyl-1-methyl-2(1H)-pyridone, and 3,5-dibenzoyl-1-methyl-2(1H)-pyridone; 3-benzoyl-1-methyl-2-(1H)-quinolone and 6-benzoyl-1-methyl-2(1H)-quinolone; and 4-benzoyl-2-methyl-1-(2H)-isoquinolone and 5-benzoyl-2-methyl-1(2H)-isoquinolone, resp.

IT 53995-93-0P

RL: PREP (Preparation)

(by Friedel-Craft acylation)

RN 53995-93-0 CAPLUS

CN 2(1H)-Quinolinone, 6-benzoyl-1-methyl- (CA INDEX NAME)

L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1963:462385 CAPLUS

DOCUMENT NUMBER: 59:62385

ORIGINAL REFERENCE NO.: 59:11514c-h,11515a TITLE: Dihydroquinoxal-2-ones

INVENTOR(S): Zellner, Hugo; Pailer, Matthias; Pruckmayr, Gerfried

PATENT ASSIGNEE(S): Donau-Pharmazie G.m.b.H.

SOURCE: 12 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

AT 228204 19630710 AT 19590703 <-PRIORITY APPLN. INFO.: AT 19590703

GI For diagram(s), see printed CA Issue.

AB New dihydroquinoxal-2-ones (I), in which R1, R2, R3, R7, and R8 are H, halogen, alkyl, OH, alkoxy, acyloxy, alkyloxy, NH2, monoalkylamino, dialkylamino, acylamino, NO2, or alkylthio groups, R4 is dialkylaminoalkyl, aminoalkyl, N-alkylpiperidyl or N-alkylmorpholyl, and R5 and R6 are H, alkyl with up to 5 C atoms, OH, acyloxy, alkyloxy, NH2, acylamino, monoalkylamino, or dialkyl amino groups, and the salts thereof are prepared by treating the resp. o-phenylene diamines with suitably substituted phenylpyruvic acids or derivs. thereof to obtain the dihydroquinoxalones, which are then aminoalkylated at the 1-N atom with an amino alc. and subsequently aminated. The compds. obtained may be converted into salts. Thus, there have been prepared: 1-(diethylaminoethyl)-3-benzyldihydroquinoxal-2-one, m. 31°; 1-(diethylaminoethy])-3-(4-

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methoxybenzyl)dihydroquinoxal-2-one; 1-(diethylaminoethyl)-3-(3,4-
dimethoxybenzyl)dihydroquinoxal-2-one, m. 192°;
1-(diethylaminoethyl)-3-(3,4-methylenedioxybenzyl)dihydroquinoxal-2-one,
light yellow oil; 1-(diethylaminoethyl)-3-(3,4-dimethoxybenzyl)-6-
chlorodihydroquinoxal-2-one, b0.5 240-6°; 6-chloro-3-(4-
methoxybenzyl)-1-diethylaminoethyldihydroquinoxal-2-one, b0.01
210°; 3-(4-nitrobenzyl)-1-diethylaminoethyldihydroquinoxal-2-one,
b0.03-0.05 \ 170-5^{\circ}; \ 3-(4-dimethylaminobenzyl)-1-
diethylaminoethyldihydroquinoxal-2-one, b0.01 200-10°;
6(7)-methoxy-3-(3,4-dimethoxybenzyl)-1-diethylaminoethyldihydroquinoxal-2-
one, b0.01 220°; 6(7)-methyl-3-(4-methoxybenzyl)-1-
diethylaminoethyldihydroquinoxal-2-one, b0.01 200°;
3-(4-chlorobenzyl)-1-diethylaminoethyldihydroquinoxal-2-one, b0.01
185-90°; 3-(4-methoxybenzyl)dihydroquinoxal-2-one, m. 198°;
3-(3,4-methylenedioxybenzyl)dihydroquinoxal-2-one, m. 220°;
6(7)-methoxy-3-benzyldihydroquinoxal-2-one, 2 isomers, m. 185 and
199°, resp.; 6(7)-methoxy-3-(4-methoxybenzyl)dihydroquinoxal-2-one,
m. 190°; 6(7)-chloro-3-(4-methoxybenzyl)dihydroquinoxal-2-one, m.
227-9°; 6(7)-nitro-3-(4-methoxybenzyl)dihydroquinoxal-2-one, m.
192-7°; 6(7)-methoxy-3-(3,4-dimethoxybenzyl)dihydroquinoxal-2-
one, m. 171^{\circ}, 6(7)-methoxy-3-(3,4-methylenedioxybenzyl)dihydroquino
xal-2-one, m. 215°; 6,7-dimethoxy-3-benzyldihydroquinoxal-2-one,
m. 275°; 3-(4-ethoxybenzyl)dihydroquinoxal-2-one, m. 196°;
3-(p-chlorobenzyl)dihydroquinoxal-2-one, m. 180° (decomposition); 3-
(p-hydroxybenzyl)dihydroquinoxal-2-one, m. 246°;
3-(4-methoxyphenyl)-\alpha-ethyldihydroguinoxal-2-one, m. 205°;
6(7)-methoxy-3-(3,4-dimethoxybenzyl)-1-diethylaminoethyldihydroquinoxal-2-
one, b0.01 220°; 3-(4-ethoxybenzyl)-1-diethylaminoethyldihydroquino
xal-2-one, m. 62^{\circ}; 6(7)-methoxy-3-benzyl-1-
diethylaminoethyldihydroquinoxal-2-one, b0.01 204-8°;
3-(4-methoxybenzyl)-1-morpholinoethyldihydroquinoxal-2-one, m.
151°; 6(7)-chloro-3-(4-methoxybenzyl)-1-
morpholinoethyldihydroquinoxal-2-one, b0.005 200°;
6(7)-methoxy-3-(3,4-methylendioxybenzyl)-1-morpholinoethyldihydroquinoxal-
2-one, m. 201°, b0.01 200-10°; 3-benzyl-1-morpholinoethyldi-
hydroquinoxal-2-one, b0.005 203°; 6(7)-chloro-3-(4-methoxybenzyl)-1-
diethylaminoethyldihydroquinoxal-2-one, b0.01 210°, m.
78-9°; 6,7-dimethoxy-3-benzyl-1-diethylaminoethyldihydroquinoxal-2-
one, b0.005 230°; 1-piperidinomethyl-3-benzyldihydroquinoxal-2-one,
m. 211-12°. The compds. are useful as analgesics; they have
papaverine- and morphine-like activity.
92868-65-0
   (Derived from data in the 7th Collective Formula Index (1962-1966))
92868-65-0 CAPLUS
2(1H)-Quinoxalinone, 5-piperonyl- (7CI) (CA INDEX NAME)
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ΙT

RN

CN

L4

ACCESSION NUMBER: 1963:403525 CAPLUS

DOCUMENT NUMBER: 59:3525

ORIGINAL REFERENCE NO.: 59:626h,627a-d

TITLE: Synthesis of quinoxalone derivatives

AUTHOR(S): Pailer, M.; Pruckmayr, G.; Zellner, H.; Zellner,

Gertraud

CORPORATE SOURCE: Univ. Vienna

SOURCE: Monatshefte fuer Chemie (1962), 93, 1005-18

CODEN: MOCMB7; ISSN: 0026-9247

DOCUMENT TYPE:

LANGUAGE:

OTHER SOURCE(S):

CASREACT 59:3525

CL. For diagram(s)

Applied CA. Lague

For diagram(s), see printed CA Issue. The synthesis of a series of substituted 3-benzylquinoxal-2-ones is described. These could be expected to possess a similar pharmacol. activity to the analogous benzimidazole derivs. of similar structure. were prepared either by condensing the corresponding phenylpyruvic acid with N-diethylaminoethyl- or N-morpholinoethyl-o-phenylenediamine, or by first preparing the quinoxolone then alkylating with diethylaminoethyl chloride [or morpholinoethyl (MA) chloride] and sodamide in absolute dioxane or with K2CO3 in absolute xylene. Similarly prepared were II (R, R1, m.p. given): H, H, 312°; OMe, H, 267.5-8.5°; H, Et2NCH2CH2, 99.5-101°. R, R1, R2, R3, R4, m.p.; H, H, H, H, H, 196°; OMe, H, H, H, H, 198°; OEt, H, H, H, H, 196°; OCH2O, , H, H, H, 220°; H, H, OMe(H), H(OMe), H, 185°; H, H, H(OMe), OMe(H), H, 200°; H, H, OMe, OMe, H, 275°; OH, H, H, H, H, 243-6°; , , , , (decomposition); OMe, OMe, Cl(H), H(Cl), H, 201-2°; OMe, H, Cl(H), H(Cl), H, 220-2°; OMe, H, H(Cl), Cl(H), H, 227-9°; NO2, H, H, H, H, 268-9°; Cl, H, H, H, H, 231°; OMe, H, NO2(H), H, (NO2), H, 192-7°; OMe, H, Me(H), H(Me), H, 202-3°; OMe, H, CO2Me(H), H(CO2Me), H, 167-8°; OMe, H, benzo, , 264°; H, H, H, H, Et2NCH2CH2, -; OMe, H, H, H, Et2NCH2CH2, 69° (HCl salt m. 188°); OMe, OMe, H, H, Et2NCH2CH2, - (HCl salt m. 192°); OCH2O, , H, H, Et2NCH2CH2, - (HCl salt m. 220°); OEt, H, H, H, Et2NCH2CH2 61°; OMe, OMe, Cl(H), H(Cl), Et2NCH2CH2, -; OMe, H, H, (Cl), Cl(H), Et2NCH2CH2, 78-9°; Cl, H, H, H, Et2NCH2CH2, 73-5°; OMe, H, Me(H), H(Me), Et2NCH2CH2, 69-70°; H, H, H, H, MA, -; OMe, H, H, H, MA, 151°; Also prepared was III; HCl salt m. 207-10°.

IT 92868-65-0

(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 92868-65-0 CAPLUS

CN 2(1H)-Quinoxalinone, 5-piperonyl- (7CI) (CA INDEX NAME)

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ACCESSION NUMBER: 1940:12844 CAPLUS

DOCUMENT NUMBER: 34:12844

ORIGINAL REFERENCE NO.: 34:1986a-i,1987a

TITLE: Nitrogen heterocycles. XLVI. 4,6-

Diaminoisophthalaldehyde. 3

AUTHOR(S): Ruggli, Paul; Frey, Hugo

SOURCE: Helvetica Chimica Acta (1939), 22, 1413-27

CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

AΒ The 3,6-dicarboxylic ester produced by the addition of 2 mols. AcCH2CO2Et to 4,6-diaminoisophthalaldehyde (I) was saponified to the free acid which was decarboxylated by heating with Cu in quinoline at 160-230° for 20 min. The resulting 2,7-dimethylbenzodipyridine (II) was converted into the hexa-Br derivative which was transformed by heating with oleum to the crude benzodipyridine-2,7-dicarboxylic acid (III). A mixture of 0.25 g. III, 2 cc. of 10% NH4OH and 2 cc. alc. was triturated, diluted with 20 cc. H2O and heated. The NH3-free product was diluted with 10 cc. H2O and boiled with 0.5 g. AgNO3 in 10 cc. H2O. The crude Ag salt (0.45 g.) was boiled with 70 cc. MeOH and 0.4 g. MeI for 1 h., filtered and concentrated to 20 cc., yielding 0.2 g. (70%) of yellow needles of di-Me benzodipyridine-2,7dicarboxylate, C16H12N2O4, m. 272° (with darkening). Decarboxylation of III gave benzodipyridine (IV); perchlorate, m. 268° (explosive on rapid heating); MeI derivative, m. above 200° (decomposition). Reduction of 0.2 g. IV in 5 cc. of boiling AmOH with 0.35 g.

Na

and recrystn. from alc. gave octahydrobenzodipyridine, m. 111.5°, identified through the di-NO and di-Ac derivs., m. 179° (decomposition) and 143°, resp. Reduction of II with Na in AmOH gave as main product a resin which was converted into a colorless crystalline octahydro-2,7dimethylbenzodipyridine diperchlorate, C14H22Cl2N2O8, m. 285-6° (decomposition). The resinous free base yielded 2 isomeric di-NO derivs., m. 164.5 and 151.5-2.0°, resp. Condensation of 0.2 g. II with 0.5 g. of p-Me2NC6H4CHO at $170-5^{\circ}$ in the presence of 10 drops of piperidine produced 0.45 g. of orange-red 2,7-bis(pdimethylaminostyryl)benzodipyridine, C32H30N4, m. about 340° (with darkening), dissolving in HCl to give violet, blue, green and yellow solns. with increasing acid concns. Condensation of II with o-C6H4(CO2Et)2 by heating in the presence of Na for 14 h. at 100 $^{\circ}$ gave a scarlet crystalline powder which on sulfonation dyed wool and silk bluish red in an acid bath. A unilateral condensation of 0.6 q. I with 6 cc. AcCH2CO2Et occurred on heating in the presence of 9 drops of piperidine for 30 min. at 170°. The impure 3-acetyl-6-formyl-7aminocarbostyril yielded yellow crystals of a pure Ac derivative, C14H12N2O4, m. $320-40^{\circ}$ (decomposition). Treatment of 1 g. I in 100 cc. alc. at 30° with 14 g. of dry OHCCHNaCO2Et, boiling for 1 h. after standing for 3 days, filtering off the brown amorphous precipitate (V), adding 1 cc. H2O and standing for 8 days gave a Na salt which was dissolved in 50 cc. H2O, acidified with 10% HCl and recrystd. from dioxane, yielding di-Et 2,6-diaminoisophthalaldiformylacetate, C18H20N2O6, m. 250°

(decomposition). V was dissolved in H2O, filtered and precipitated with dilute HCl.

The amorphous product (0.06 g.) was decarboxylated by heating in vacuo with 0.3 g. BaO and 0.5 g. Cu at 150° to yield a bright yellow sublimate of IV. Condensation of I with excess cyclohexanone in the presence of piperidine produced 2,3,6,7-bis (tetramethylene)-benzodipyridine, C20H20N2, m. 250-1° (with darkening); dipicrate, m. 195° (decomposition). A mixture of 8 g. I in 150 cc. alc., 24 cc. PhCH2CN and 12.5 cc. of 30% NaOH was heated for 30 min. on the steam bath. Working up and purification through the di-HCl salt gave a free base (VI), C24H18N4, m. 301°; tetra-Ac derivative, C32H26N4O4, m. 238.5-9.5° (decomposition). Saponification of VI with HCl produced a carboxyl derivative, C24H18N2O3, which gave a Na salt and a mono-Ac derivative, m. 365°. Condensation of 4 g. of 4,6-dinitroisophthalaldehyde with

 $8.4~\rm g.$ of dry PhCH(Na)CO2H by heating with $34~\rm cc.$ Ac20 and $1.2~\rm g.$ ZnCl2 for 40 h. at 80° gave a powdery dicarboxylic acid which was esterified through the Ag salt to di-Me 4,6-dinitroisophthalalbis(phenylac etate), C26H20N2O8, m. 152.5-3.5°. Condensation of methazonic acid (VII) with o-H2NC6H4CHO yields 3-nitroquinoline and similarly a cold mixture of VII and I in the presence of a min. of HCl gave 20% of yellow-orange needles of a compound C16H14N6O5, m. 290° (decomposition), of undetd. composition

IT 855762-40-2P, 6-Quinolineacrylic acid, 7-amino-1,2-dihydro-2-oxo- α ,3-diphenyl- 855762-42-4P, 6-Quinolineacrylic acid, 7-acetamido-1,2-dihydro-2-oxo- α ,3-diphenyl-

RN 855762-40-2 CAPLUS

CN Benzeneacetic acid, α -[(7-amino-1,2-dihydro-2-oxo-3-phenyl-6-quinolinyl)methylene]- (CA INDEX NAME)

RN 855762-42-4 CAPLUS

CN Benzeneacetic acid, α -[[7-(acetylamino)-1,2-dihydro-2-oxo-3-phenyl-6-quinolinyl]methylene]- (CA INDEX NAME)

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